The Unrestricted Local Properties as a Useful Tool for Nanoelectronics

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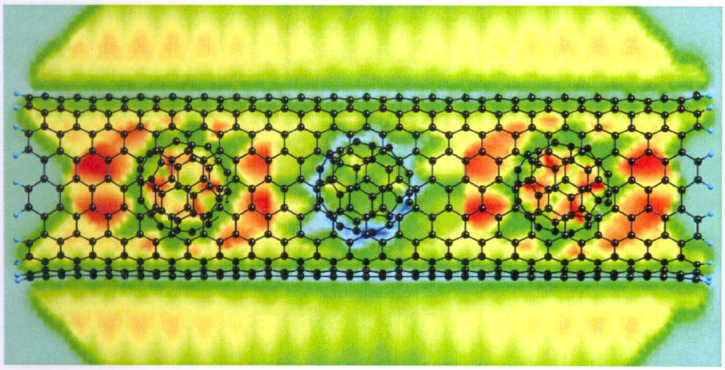
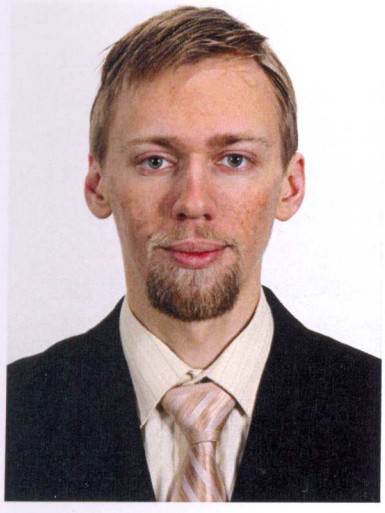


The potential of the local electron affinity (EAL) is now recognized for application in modeling electronic devices [1], although both EAL and the local ionization energy (IEL) have been extensively used for drug design much longer. However, closed-shell species are usually modelled in the latter application and only restricted formulations of EAL and IEL were used therefore for molecular species. Since electrons and holes are generated in electronic devices, we have recently extended EAL and IEL to the unrestricted case [2]. We have demonstrated on example of carbon peapod that unrestricted EAL and IEL are especially useful for understanding how ambipolar transistors work [2]. We recommend the use of the unrestricted EAL and IEL also for modeling devices built from closed-shell molecular species because of extremely large RHF->UHF instability for such systems. Taking into account relatively large size of nanosystems this approach was implemented into the semiempirical framework that makes it computationally fast tool for studying nanoelectronic properties.

[1] C. M. Jäger et al. J. Am. Chem. Soc. 2013, 135, 4893-4900
[2] P. O. Dral, J. Mol. Model. 2014, 20, 2134



Pavlo Dral did the graduate studies in chemical technology and engineering at the National Technical University of Ukraine "Kiev Polytechnic Institute" (KPI) with Prof. Dr. Andrey A. Fokin and in molecular nanoscience at the Friedrich-Alexander-University Erlangen-Nuremberg (FAU) with Prof. Dr. Timothy Clark in 2008–2010. Pavlo Dral graduated his doctoral studies with Prof. Dr. Timothy Clark in the Computer Chemistry Center at the FAU in 2013. In 2013 Pavlo Dral joined the group of Prof. Dr. Walter Thiel in the Max-Planck-Institut für Kohlenforschung. Pavlo Dral received several scholarships including stipend within the Bavarian Elite Aid Program and conference awards. His research interests include development and application of quantum chemical and machine learning methods for computer chemistry.